

The shear modulus of glasses: results from the full replica symmetry breaking solution

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We compute the shear modulus of amorphous hard spheres, using the exact solution in infinite spatial dimensions that has been developed recently. We characterize the behavior of this observable in the whole phase diagram, and in particular around the glass and jamming transitions. Our results are consistent with other theoretical approaches, that are unified within this general picture, and they are also consistent with numerical and experimental results. Furthermore, we discuss some properties of the out-of-equilibrium dynamics after a deep quench close to the jamming transition, and we show that a combined measure of the shear modulus and of the mean square displacement allows one to probe experimentally the complex structure of phase space predicted by the full replica symmetry breaking solution.

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I. INTRODUCTION

Amorphous hard spheres, that are a good model for colloidal glasses, molecular glasses, and granular media [1–3], display a very complex rheological behavior, controlled by two distinct “critical” points: the glass transition and the jamming transition [2, 4]. At densities below the glass transition, the system is liquid, hence it can flow and its shear modulus vanishes. At the glass transition, the system acquires a finite rigidity through a discontinuous transition at which the shear modulus jumps to a finite value [5, 6]. Simultaneously the yield stress may also exhibit a similar discontinuous transition [4, 7]. It is important to stress that at densities slightly above the glass transition, rigidity has an *entropic* origin, as in a hard sphere crystal [4, 8]. In fact, at zero temperatures, the spheres have enough room to fit in space without touching, hence they do not interact and the system is loose. At any finite temperature, however, the spheres vibrate and collide, so they exchange momentum, giving rise to an effective interaction that makes the system rigid [9]. Both the pressure and the shear modulus are therefore proportional to temperature in this region of density. Upon further compression, the system reaches a “random close packing” or “jamming” density, at which infinitely hard particles cannot be compressed anymore [10–13]. Above this density, the spheres cannot fit in space without being “squeezed” by their neighbors, and rigidity and pressure acquire a *mechanical* origin, being due to a direct interaction between the particles [4, 14]. Both pressure and the shear modulus, therefore, have a finite zero-temperature limit in this region.

The interplay of the jamming and glass transitions gives rise to complex flow curves in the packing fraction-temperature (φ, T) plane, which have been recently characterized in full details [4]. Concerning the behavior of the shear modulus μ , two main qualitative observations have been made. First, the shear modulus jumps discontinuously at the glass transition; secondly, it has a critical behavior around the jamming transition at φ_j . In fact, it diverges as $\mu \sim T(\varphi_j - \varphi)^{-\kappa}$ for hard spheres when $\varphi \rightarrow \varphi_j^-$, with κ close to $3/2$ [9], and it vanishes as $\mu \sim (\varphi - \varphi_j)^{\kappa'}$ for soft harmonic spheres when $\varphi \rightarrow \varphi_j^+$ and $T = 0$, with κ' close to $1/2$ [13, 15]. For hard spheres, the exponents κ has been related to other exponents that characterize criticality at the jamming transition [16], whereas for soft spheres the prediction that $\kappa' = 1/2$ was made using different approximations [15, 17]. Remarkably, despite the fact that both the glass and the jamming transition happen out-of-equilibrium, hence at protocol-dependent densities, the critical properties around these transitions are universal and independent of the protocol, for a wide range of reasonable preparation protocols [2, 4, 16, 18, 19].

Constructing a first principle theory able to describe the complex rheological properties of these systems is a difficult task. One of the most successful theories is Mode-Coupling Theory (MCT) [20], that is based on an approximate set of dynamical equations, and can describe well the rheological properties around the glass transition [5, 7]. However, MCT does not provide good results deep in the glass phase and in particular it fails to describe correctly the jamming transition [21]. Another first-principle approach to glass physics is based on the assumption that glasses are long-lived metastable states, and can be described by a restricted equilibrium thermodynamics. Concrete computations can then be done using replicas, and have been usually done within the so-called “1-step replica symmetry breaking” (1RSB) scheme [2, 22]. This method has been applied to describe the rigidity of structural glasses, including the hard sphere systems [6, 23–25], and provides good qualitative and quantitative results for the shear modulus, but in the simplest 1RSB scheme it fails to predict the exponents κ and κ' correctly [24, 25]. Both the MCT and the replica approach are thought to be part of the more general Random First Order Transition (RFOT) scenario for the glass transition [26–28].

Following a well-established tradition in theoretical physics [29], in [30–32] a new approach was adopted by solving exactly the hard sphere model in the limit of $d \rightarrow \infty$, in which the RFOT scenario is exactly realized [26]. In particular, in [32] it was shown that in addition to the glass and jamming transitions, a new transition takes place deep in the glass phase and before jamming occurs. This so-called Gardner transition is a transition where the 1RSB structure changes into a full replica symmetry breaking (fullRSB) one [33, 34]. Physically, this corresponds to a splitting of glass basins into a complex hierarchy of subbasins, akin to the one of the Sherrington-Kirkpatrick model. This structure has been described in details in the literature [34]. In [32] it was shown that this exact solution predicts a phase diagram which is in very good qualitative agreement with the one observed in numerical simulations and experiments, and in particular it gives correct *analytical* predictions for the critical exponents that characterize the jamming transition.

The aim of this paper is to extend the analysis of [32] to describe the rheological properties of hard spheres in the limit $d \rightarrow \infty$, and in particular to compute the shear modulus. Our main results are: (i) at the dynamic glass transition φ_d , the shear modulus μ jumps discontinuously to a finite value, and at densities slightly above the transition it displays a square-root singularity $\mu \sim \mu_d + C(\varphi - \varphi_d)^{1/2}$; (ii) the critical properties around the jamming transition φ_j are the ones described above, with $\mu \sim T(\varphi_j - \varphi)^{-\kappa}$ for $\varphi \rightarrow \varphi_j^-$ with $\kappa = 1.41575$, and $\mu \sim (\varphi - \varphi_j)^{\kappa'}$ for $\varphi \rightarrow \varphi_j^+$ and $T = 0$ with $\kappa' = 2 - \kappa = 0.58425$; (iii) we derive predictions for the out-of-equilibrium dynamics after a deep quench close to the jamming transition that are direct consequences of the fullRSB structure. Our approach unifies, in a well controlled setting, several theoretical approaches such as MCT [5, 7, 21] and effective medium approaches [9, 15, 16].

The qualitative phase diagram is consistent with numerical results [4], and the predicted critical exponents also agree well with numerical results [4, 9, 13, 25]. Moreover, the present approach can be extended to provide quantitative predictions for non-universal quantities in finite dimensions [2, 6, 22]. Despite all this, some problems remain open and we discuss them in the conclusions.

II. SHEARING THE MOLECULAR LIQUID

A. General formulation

In the following, we consider a system of N identical particles in a cubic d dimensional volume V , with density $\rho = N/V$. Particles interact through a two-body potential $v(r)$, and in most cases this will be the hard sphere potential with diameter D , but to keep the discussion more general, we consider also a generic soft potential with range D and temperature $T = 1/\beta$. We define the packing fraction $\varphi = \rho V_d (D/2)^d$, where V_d is the volume of a d -dimensional sphere of unit radius [2], and a scaled packing fraction $\hat{\varphi} = \rho V_d D^d / d = 2^d \varphi / d$. We consider first the thermodynamic limit $N \rightarrow \infty$, and then the limit $d \rightarrow \infty$.

A general approach to compute properties of glasses through a “cloned liquid” replica method has been presented in [22], and applied to the computation of the shear modulus in [6, 23]. To keep this paper reasonably short, we cannot reproduce this construction here. We therefore assume that the reader is familiar with (i) the general formalism of the replica method of spin glasses, including the 1-step replica symmetry breaking (1RSB) and full replica symmetry breaking (fullRSB) schemes, reviewed e.g. in [34, 35]; (ii) the “cloned liquid” construction to compute properties of glasses, originally introduced in [36, 37] and reviewed in [22], including its application to compute the shear modulus [6]; (iii) its application to hard sphere systems, reviewed in [2], and in particular the structure of the 1RSB solution in the limit $d \rightarrow \infty$ [2, Sec.VI]; (iv) the construction of a fullRSB solution for hard spheres in $d \rightarrow \infty$ and the associated phase diagram, obtained in [30–32].

To describe glassy states, we consider m identical replicas of the original system [36]. To describe the fullRSB structure, we follow the results and the notations of [32], and we assume that the m replicas all belong to one of the largest metabasins, in such a way that their mean square displacement is at most $\hat{\Delta}_1$. As a consequence, the replicas form a *molecular liquid* in which each molecule contains one particle of each of the replicas.

Each molecule is described by a set of m coordinates $\vec{x} = \{x_1 \cdots x_m\}$, where x_a are d -dimensional vectors. Following [6, 23], we apply a strain γ_a to replica a , which is obtained by deforming linearly the volume in which the system is contained. We call x'_μ , with $\mu = 1, \dots, d$, the coordinates in the original reference frame, in which the strain is applied. In this frame, the cubic volume is deformed because of strain. To remove this undesirable feature, we introduce new coordinates x_μ of a “strained” frame in which the volume is brought back to a cubic shape. If the strain is applied along direction $\mu = 2$, then for replica a all the coordinates are unchanged, $x_{a\mu} = x'_{a\mu}$, except the first one which is changed according to

$$x'_{a1} = x_{a1} + \gamma_a x_{a2} , \quad x_{a1} = x'_{a1} - \gamma_a x'_{a2} . \quad (1)$$

Let us call $S(\gamma_a)$ the matrix such that $x'_a = S(\gamma_a)x_a$. In the original frame (where the volume is deformed by strain), two particles of replica a interact with the potential $v(|x'_a - y'_a|)$. If we change variable to the strained frame (where the volume is not deformed), the interaction is

$$v_{\gamma_a}(x_a - y_a) = v(|S(\gamma_a)(x_a - y_a)|) . \quad (2)$$

An important remark is that $\det S(\gamma) = 1$ meaning that the simple strain defined above does not change the volume and thus the average density $\rho = N/V$ of the system.

In $d \rightarrow \infty$, we keep only the first non-trivial term of the virial series [2, 30, 38]. Using the coordinates of the strained frame, the system is translationally invariant in the usual way and, following the same steps and notations of [30], we can write the free energy of the replicated liquid as

$$\begin{aligned} -\beta N F(\{\gamma_a\}) &= \int d\vec{x} \rho(\vec{x}) [1 - \log \rho(\vec{x})] + \frac{1}{2} \int d\vec{x} d\vec{y} \rho(\vec{x}) \rho(\vec{y}) f_{\{\gamma_a\}}(\vec{x} - \vec{y}) \\ &= V \int \mathcal{D}\vec{u} \rho(\vec{u}) [1 - \log \rho(\vec{u})] + \frac{V}{2} \int \mathcal{D}\vec{u} \mathcal{D}\vec{v} \rho(\vec{u}) \rho(\vec{v}) \bar{f}_{\{\gamma_a\}}(\vec{u} - \vec{v}) , \end{aligned} \quad (3)$$

where $X = m^{-1} \sum_a x_a$ is the center of mass of a molecule, $u_a = x_a - X$ is the displacement of replica a in the molecule, the Mayer function is

$$f_{\{\gamma_a\}}(\vec{x} - \vec{y}) = -1 + \prod_{a=1}^m e^{-\beta v(|S(\gamma_a)(x_a - y_a)|)} = f(\{S(\gamma_a)(x_a - y_a)\}) , \quad (4)$$

$f(\bar{x} - \bar{y})$ is the usual Mayer function that was considered in [30], and $\bar{f}_{\{\gamma_a\}}(\bar{u} - \bar{v}) = \int dX f_{\{\gamma_a\}}(X + \bar{u} - \bar{v})$ is the translationally averaged Mayer function as in [30].

Following [6, 23], we want to develop the free energy for small γ_a , and we define

$$F(\{\gamma_a\}) = F(\{0\}) + \sum_{a=1}^m \sigma_a \gamma_a + \frac{1}{2} \sum_{a,b}^{1,m} \mu_{ab} \gamma_a \gamma_b + \dots \quad (5)$$

which defines the shear modulus matrix μ_{ab} , whose physical interpretation will be discussed later.

B. Replicated Mayer function in presence of strain

Clearly, the strain γ_a enters only in the second term of Eq. (3), that represents the mean field density-density interaction, and for this reason we call it the “interaction term” [30]. We shall therefore repeat the steps of [30, Sec. 5] in presence of the strain.

We specialize to hard spheres. Taking into account translational invariance following the same steps as in [30], we obtain a modified Mayer function that reads

$$\bar{f}_{\{\gamma_a\}}(\bar{u}) = \int dX \left\{ -1 + \prod_{a=1}^m \theta(|S(\gamma_a)(X + u_a)| - D) \right\} = - \int dX \theta(D - \min_a |S(\gamma_a)(X + u_a)|) . \quad (6)$$

This function is integrated over $\bar{u} - \bar{v}$ in Eq. (3), where \bar{u} and \bar{v} are extracted from the density distribution $\rho(\bar{u})$. Here we shift $u_a - v_a \rightarrow u_a$. The m vectors u_a define an m -dimensional plane in the d -dimensional space, and it is reasonable to assume that this plane is orthogonal to the strain directions $\mu = 1, 2$ with probability going to 1 for $d \rightarrow \infty \gg m$. Hence, the vector X can be decomposed in a two dimensional vector $\{X_1, X_2\}$ parallel to the strain plane, a $(d - m - 2)$ -component vector X_\perp , orthogonal to the plane $\mu = 1, 2$ and to the plane defined by u_a , and a m -component vector X_\parallel parallel to that plane. Defining Ω_d as the d -dimensional solid angle and recalling that $V_d = \Omega_d/d$, and following the same steps as in [30, Sec. 5], we have

$$\begin{aligned} \bar{f}_{\{\gamma_a\}}(\bar{u}) &= - \int dX \theta(D^2 - \min_a |S(\gamma_a)(X + u_a)|^2) \\ &= - \int dX_1 dX_2 d^m X_\parallel d^{d-m-2} X_\perp \theta(D^2 - \min_a \{(X_1 + \gamma_a X_2)^2 + X_2^2 + |X_\parallel + u_a|^2 + |X_\perp|^2\}) \\ &= -\Omega_{d-m-2} \int dX_1 dX_2 d^m X_\parallel \int_0^\infty dx x^{d-m-3} \theta(D^2 - x^2 - \min_a \{(X_1 + \gamma_a X_2)^2 + X_2^2 + |X_\parallel + u_a|^2\}) \\ &= -\Omega_{d-m-2} \int dX_1 dX_2 d^m X_\parallel \int_0^{\sqrt{D^2 - \min_a \{(X_1 + \gamma_a X_2)^2 + X_2^2 + |X_\parallel + u_a|^2\}}} dx x^{d-m-3} \\ &= -V_{d-m-2} \int dX_1 dX_2 d^m X_\parallel \Theta_{d-m-2}(D^2 - \min_a \{(X_1 + \gamma_a X_2)^2 + X_2^2 + |X_\parallel + u_a|^2\}) \end{aligned} \quad (7)$$

where we defined the function [30]

$$\Theta_n(x) = x^{n/2} \theta(x) . \quad (8)$$

It has been shown in [30] that the region where $\bar{f}_{\{\gamma_a\}}(\bar{u})$ has a non-trivial dependence on the u_a is where $u_a \sim 1/\sqrt{d}$. Hence we define $u_a = x_a D/\sqrt{d}$, $X_{1,2} = \zeta_{1,2} D/\sqrt{d}$ and $X_\parallel = \epsilon D/\sqrt{d}$. Using that $\lim_{n \rightarrow \infty} \Theta_n(1 + y/n) = e^{y/2}$, and that for large d and finite k we have $V_{d-k}/V_d \sim d^{k/2}/(2\pi)^{k/2}$, we have

$$\begin{aligned} \bar{f}_{\{\gamma_a\}}(\bar{u}) &= -\frac{V_{d-m-2}}{V_d} \frac{V_d D^d}{d^{(m+2)/2}} \int d\zeta_1 d\zeta_2 d^m \epsilon \Theta_{d-m-2} \left(1 - \frac{1}{d} \min_a \{(\zeta_1 + \gamma_a \zeta_2)^2 + \zeta_2^2 + |\epsilon + x_a|^2\} \right) \\ &\sim -V_d D^d \int \frac{d\zeta_1 d\zeta_2 d^m \epsilon}{(2\pi)^{(m+2)/2}} e^{-\frac{1}{2} \min_a \{(\zeta_1 + \gamma_a \zeta_2)^2 + \zeta_2^2 + |\epsilon + x_a|^2\}} \equiv -V_d D^d \mathcal{F}_{\{\gamma_a\}}(\bar{x}) , \end{aligned} \quad (9)$$

where the function \mathcal{F} has been introduced following [30, 31].

We can then follow the same steps as in [31, Sec.V C] to write

$$\begin{aligned}
\mathcal{F}_{\{\gamma_a\}}(\bar{x}) &= \int \frac{d\zeta_1 d\zeta_2 d^m \epsilon}{(2\pi)^{(m+2)/2}} e^{-\frac{1}{2} \min_a \{(\zeta_1 + \gamma_a \zeta_2)^2 + \zeta_2^2 + |\epsilon + x_a|^2\}} = \int \frac{d\zeta_1 d\zeta_2 d^m \epsilon}{(2\pi)^{(m+2)/2}} \lim_{n \rightarrow 0} \left(\sum_{a=1}^m e^{-\frac{1}{2n} [(\zeta_1 + \gamma_a \zeta_2)^2 + \zeta_2^2 + |\epsilon + x_a|^2]} \right)^n \\
&= \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m; \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} \int \frac{d\zeta_1 d\zeta_2 d^m \epsilon}{(2\pi)^{(m+2)/2}} e^{-\sum_a \frac{n_a}{2n} [(\zeta_1 + \gamma_a \zeta_2)^2 + \zeta_2^2 + |\epsilon + x_a|^2]} \\
&= \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m; \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} e^{-\frac{1}{2} \sum_{a=1}^m \frac{n_a}{n} |x_a|^2 + \frac{1}{2} \sum_{a,b}^{1,m} \frac{n_a n_b}{n^2} x_a \cdot x_b} \int \frac{d\zeta_1 d\zeta_2}{2\pi} e^{-\sum_a \frac{n_a}{2n} [(\zeta_1 + \gamma_a \zeta_2)^2 + \zeta_2^2]} \\
&= \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m; \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} e^{-\frac{1}{4} \sum_{a,b}^{1,m} \frac{n_a n_b}{n^2} (x_a - x_b)^2} \int \frac{d\zeta}{\sqrt{2\pi}} e^{-\frac{\zeta^2}{2} [1 + \frac{1}{2} \sum_{ab} \frac{n_a n_b}{n^2} (\gamma_a - \gamma_b)^2]} \\
&= \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m; \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} e^{-\frac{1}{4} \sum_{a,b}^{1,m} \frac{n_a n_b}{n^2} \Delta_{ab}} \int \frac{d\zeta}{\sqrt{2\pi}} e^{-\frac{\zeta^2}{2} [1 + \frac{1}{2} \sum_{ab} \frac{n_a n_b}{n^2} (\gamma_a - \gamma_b)^2]} ,
\end{aligned} \tag{10}$$

where we introduced the matrix $\hat{\Delta}$ of mean square displacements between replicas

$$\Delta_{ab} = (x_a - x_b)^2 = \frac{d}{D^2} (u_a - u_b)^2 . \tag{11}$$

We should now recall that in Eq. (3) the Mayer function is evaluated in $\bar{u} - \bar{v}$, hence after rescaling the function \mathcal{F} is evaluated in $\bar{x} - \bar{y}$. For $d \rightarrow \infty$, the interaction term is dominated by a saddle point on \bar{u} and \bar{v} , such that $(x_a - x_b)^2 = (y_a - y_b)^2 = \Delta_{ab}$ and $x_a \cdot y_b = 0$ [30–32], hence $(x_a - y_a - x_b + y_b)^2 = (x_a - x_b)^2 + (y_a - y_b)^2 = 2\Delta_{ab}$. We therefore obtain at the saddle point

$$\begin{aligned}
\mathcal{F}_{\{\gamma_a\}}(\hat{\Delta}) &= \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m; \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} e^{-\frac{1}{2} \sum_{a,b}^{1,m} \frac{n_a n_b}{n^2} \Delta_{ab}} \int \frac{d\zeta}{\sqrt{2\pi}} e^{-\frac{\zeta^2}{2} [1 + \frac{1}{2} \sum_{ab} \frac{n_a n_b}{n^2} (\gamma_a - \gamma_b)^2]} \\
&= \int \frac{d\zeta}{\sqrt{2\pi}} e^{-\frac{\zeta^2}{2}} \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m; \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} e^{-\frac{1}{2} \sum_{a,b}^{1,m} \frac{n_a n_b}{n^2} (\Delta_{ab} + \frac{\zeta^2}{2} (\gamma_a - \gamma_b)^2)} \\
&= \int \frac{d\zeta}{\sqrt{2\pi}} e^{-\frac{\zeta^2}{2}} \mathcal{F} \left(\Delta_{ab} + \frac{\zeta^2}{2} (\gamma_a - \gamma_b)^2 \right) ,
\end{aligned} \tag{12}$$

where $\mathcal{F}(\hat{\Delta})$ is the interaction function in absence of strain, that was used in [30–32].

C. Replicated entropy in presence of strain

Collecting all terms, we obtain for the replicated free energy

$$s(\hat{\Delta}, \{\gamma_a\}) = -\beta F(\hat{\Delta}, \{\gamma_a\}) = s_{\text{ent}}(\hat{\Delta}) - \frac{d\hat{\varphi}}{2} \mathcal{F}_{\{\gamma_a\}}(\hat{\Delta}) = s_{\text{ent}}(\hat{\Delta}) - \frac{d\hat{\varphi}}{2} \int \frac{d\zeta}{\sqrt{2\pi}} e^{-\frac{\zeta^2}{2}} \mathcal{F} \left(\Delta_{ab} + \frac{\zeta^2}{2} (\gamma_a - \gamma_b)^2 \right) , \tag{13}$$

where the “entropic” or ideal gas term $s_{\text{ent}}(\hat{\Delta})$ does not depend on strain and has been computed in [30–32].

Eq. (13) has two important properties. First, the correction in γ_a is clearly quadratic, hence according to Eq. (5) we have $\sigma_a = 0$ for all a . We will show below that σ_a is the average stress of glassy states under a small strain γ_a . But because of disorder, taking the average over all glasses, the average stress vanishes at $\gamma_a = 0$, hence $\sigma_a = 0$. Second, a uniform strain $\gamma_a = \gamma$ has no effect on the replicated system, which is correct because the molecules are always in the liquid phase [6, 22].

The fact that the correction is quadratic has another important consequence: to obtain the shear modulus matrix, we can formally consider $(\gamma_a - \gamma_b)^2$ as a small parameter and take the first order correction in this parameter. This is important, because the matrix $\hat{\Delta}$ has to be determined by solving the variational equations $\frac{\partial s}{\partial \Delta_{ab}} = 0$ and therefore

it also depends on $\{\gamma_\alpha\}$. However, at linear order, the dependence of $\hat{\Delta}$ on $\{\gamma_\alpha\}$ is irrelevant to compute the shear modulus matrix, precisely because $\frac{\partial s}{\partial \Delta_{ab}} = 0$ identically¹.

D. The shear modulus matrix

Eq. (13) is an exact result for $d \rightarrow \infty$ and it allows one to compute all the terms in the expansion for small γ_a , that contain the linear and non-linear responses to an applied strain. In this paper, however, we focus on the linear response defined by the matrix μ_{ab} introduced in Eq. (5).

Because the matrix $\hat{\Delta}$ is symmetric, we consider that $\mathcal{F}(\hat{\Delta})$ is a function of $\Delta_{a < b}$ only, and the derivative $\frac{\partial \mathcal{F}}{\partial \Delta_{ab}}$ is defined as the variation of $\mathcal{F}(\hat{\Delta})$ under a variation of Δ_{ab} , that therefore also induces an identical variation of Δ_{ba} . With this convention, we have at the lowest order

$$-\beta F(\hat{\Delta}, \{\gamma_a\}) = -\beta F(\hat{\Delta}) - \frac{d\hat{\varphi}}{4} \sum_{a < b} \frac{\partial \mathcal{F}}{\partial \Delta_{ab}} (\gamma_a - \gamma_b)^2, \quad (14)$$

and rearranging the terms it is easy to see that

$$\beta \mu_{ab} = \frac{d}{2} \hat{\varphi} \left[\delta_{ab} \sum_{c(\neq a)} \frac{\partial \mathcal{F}}{\partial \Delta_{ac}} - (1 - \delta_{ab}) \frac{\partial \mathcal{F}}{\partial \Delta_{ab}} \right]. \quad (15)$$

Note that from Eq. (15) it is clear that $\sum_b \mu_{ab} = 0$, as it should be because the molecular liquid is in fact a liquid [6].

E. The fullRSB structure

We can now insert in Eq. (15) the fullRSB structure of the matrix $\hat{\Delta}$, as described in [32]. Let us define the matrix $I_{ab}^{m_i}$, which has elements equal to 1 in blocks of size m_i around the diagonal, and zero otherwise. Then, using the notations of [32], and noting that $I_{ab}^{m_k=1} = \delta_{ab}$, one has for a k RSB matrix:

$$\Delta_{ab} = \sum_{i=1}^k \hat{\Delta}_i (I_{ab}^{m_{i-1}} - I_{ab}^{m_i}) = \sum_{i=0}^{k-1} (\hat{\Delta}_{i+1} - \hat{\Delta}_i) I_{ab}^{m_i} - \hat{\Delta}_k \delta_{ab}. \quad (16)$$

Correspondingly, one has

$$\frac{\partial \mathcal{F}}{\partial \Delta_{ab}} = \sum_{i=1}^k \frac{2}{m(m_{i-1} - m_i)} (I_{ab}^{m_{i-1}} - I_{ab}^{m_i}) \frac{\partial \mathcal{F}}{\partial \hat{\Delta}_i}, \quad (17)$$

and therefore, introducing $J_{ab}^{m_i} = I_{ab}^{m_i} - m_i \delta_{ab}$, we have

$$\beta \mu_{ab} = d \hat{\varphi} \left[\sum_{i=1}^k \frac{1}{m(m_{i-1} - m_i)} (J_{ab}^{m_i} - J_{ab}^{m_{i-1}}) \frac{\partial \mathcal{F}}{\partial \hat{\Delta}_i} \right]. \quad (18)$$

¹ This argument can be illustrated as follows. Suppose that $s(\hat{\Delta}, \varepsilon)$ depends on a single parameter ε . The matrix $\hat{\Delta}_\varepsilon$ is the solution of the equation

$$\frac{\partial s}{\partial \Delta_{ab}} = 0.$$

Hence, the linear variation of the entropy with respect to ε is

$$\frac{ds}{d\varepsilon}(\hat{\Delta}_\varepsilon, \varepsilon) = \frac{\partial s}{\partial \varepsilon}(\hat{\Delta}_\varepsilon, \varepsilon) + \sum_{ab} \frac{\partial s}{\partial \Delta_{ab}}(\hat{\Delta}_\varepsilon, \varepsilon) \frac{d\Delta_{ab, \varepsilon}}{d\varepsilon} = \frac{\partial s}{\partial \varepsilon}(\hat{\Delta}_\varepsilon, \varepsilon)$$

precisely because of the variational condition. Hence in the limit $\varepsilon \rightarrow 0$ one has

$$\lim_{\varepsilon \rightarrow 0} \frac{ds}{d\varepsilon}(\hat{\Delta}_\varepsilon, \varepsilon) = \frac{\partial s}{\partial \varepsilon}(\hat{\Delta}_{\varepsilon=0}, \varepsilon = 0),$$

and the dependence of $\hat{\Delta}_\varepsilon$ on ε can be ignored, one only has to compute the partial derivative with respect to ε and evaluate the result using the unperturbed $\hat{\Delta}$.

Using the results in [32, Eqs. (45) and (61)], we have

$$\frac{\partial \mathcal{F}}{\partial \widehat{\Delta}_i} = \int_{-\infty}^{\infty} dh e^h \frac{d}{dh} \frac{\partial g(m, h)}{\partial \widehat{\Delta}_i} = \frac{m(m_i - m_{i-1})}{2} \int_{-\infty}^{\infty} dh e^h \frac{d}{dh} N_i(m, h) , \quad (19)$$

and following the same procedure as in [32, Eqs. (66)-(70)], we obtain

$$\frac{\partial \mathcal{F}}{\partial \widehat{\Delta}_i} = \frac{m(m_{i-1} - m_i)}{2} e^{-\widehat{\Delta}_1/2} \int_{-\infty}^{\infty} dh P(m_i, h) f'(m_i, h)^2 , \quad (20)$$

and

$$\beta \mu_{ab} = \frac{d}{2} \widehat{\varphi} \sum_{i=1}^k (J_{ab}^{m_i} - J_{ab}^{m_{i-1}}) e^{-\widehat{\Delta}_1/2} \int_{-\infty}^{\infty} dh P(m_i, h) f'(m_i, h)^2 . \quad (21)$$

Using then the changes of notations of [32, Sec. IV A], we obtain

$$\beta \mu_{ab} = \frac{d}{2} \widehat{\varphi} \sum_{i=1}^k (J_{ab}^{m_i} - J_{ab}^{m_{i-1}}) \frac{1}{m^2} \int_{-\infty}^{\infty} dh e^h \widehat{P}(y_i, h) \widehat{f}'(y_i, h)^2 = d \sum_{i=1}^k (J_{ab}^{m_i} - J_{ab}^{m_{i-1}}) \frac{\widehat{\kappa}_i}{m^2} . \quad (22)$$

Recalling that $m_k = 1$, $I_{ab}^{m_k} = \delta_{ab}$, and using [32, Eq. (113)], we can rearrange the expression above as

$$\begin{aligned} \beta \widehat{\mu}_{ab} &= \frac{\beta \mu_{ab}}{d} = \frac{1}{m^2} \left[\widehat{\kappa}_k + \sum_{i=1}^k (m_{i-1} - m_i) \widehat{\kappa}_i \right] I_{ab}^{m_k} + \sum_{i=1}^{k-1} \frac{\widehat{\kappa}_i - \widehat{\kappa}_{i+1}}{m^2} I_{ab}^{m_i} - \frac{\widehat{\kappa}_1}{m^2} I_{ab}^{m_0} \\ &= \frac{1}{m \widehat{\gamma}_k} I_{ab}^{m_k} + \sum_{i=1}^{k-1} \frac{1}{m m_i} \left(\frac{1}{\widehat{\gamma}_i} - \frac{1}{\widehat{\gamma}_{i+1}} \right) I_{ab}^{m_i} - \frac{1}{m^2 \widehat{\gamma}_1} I_{ab}^{m_0} . \end{aligned} \quad (23)$$

III. PHYSICAL INTERPRETATION: DECOMPOSITION OF THE GIBBS MEASURE OVER PURE STATES

We now derive a physical interpretation of Eq. (23) by means of the decomposition of the equilibrium Gibbs measure over the set of pure states, each representing a glassy state. Since this decomposition has been discussed in details in the literature [2, 6, 22, 34], we assume that the reader is familiar with the construction. For simplicity, we discuss here the 2RSB case only, by generalizing the 1RSB discussion of [6]: the generalization to k RSB and fullRSB is straightforward.

A. Decomposition of thermodynamic averages over pure glassy states

The 2RSB ansatz describes a system whose glassy states are arranged as follows. Each glass state (or basin) is labeled by an index α_1 and has a free energy per particle f_{α_1} . These states are organized in “metabasins”. Each metabasin is labeled by an index α_0 and contains a set of glassy basins. We say that $\alpha_1 \in \alpha_0$ if basin α_1 belongs to metabasin α_0 . A basin α_1 has a weight within its metabasin α_0 given by

$$w_{\alpha_1|\alpha_0} = \frac{e^{-\beta N m_1 f_{\alpha_1}}}{\sum_{\alpha_1 \in \alpha_0} e^{-\beta N m_1 f_{\alpha_1}}} = \frac{e^{-\beta N m_1 f_{\alpha_1}}}{e^{-\beta N m_1 f_{\alpha_0}}} , \quad (24)$$

where T/m_1 is the effective temperature associated to the distribution of basins within metabasins, and we defined

$$Z_{\alpha_0} = e^{-\beta N m_1 f_{\alpha_0}} = \sum_{\alpha_1 \in \alpha_0} e^{-\beta N m_1 f_{\alpha_1}} \quad (25)$$

as the partition function restricted to metabasin α_0 . The weight of a metabasin in the total Gibbs measure is given by

$$w_{\alpha_0} = \frac{e^{-\beta N m_0 f_{\alpha_0}}}{\sum_{\alpha_0} e^{-\beta N m_0 f_{\alpha_0}}} = \frac{(Z_{\alpha_0})^{\frac{m_0}{m_1}}}{Z} , \quad (26)$$

where T/m_0 is the effective temperature associated to the distribution of metabasins, and the total partition function of the system is

$$Z = \sum_{\alpha_0} e^{-\beta N m_0 f_{\alpha_0}} = \sum_{\alpha_0} (Z_{\alpha_0})^{\frac{m_0}{m_1}} = \sum_{\alpha_0} \left(\sum_{\alpha_1 \in \alpha_0} e^{-\beta N m_1 f_{\alpha_1}} \right)^{\frac{m_0}{m_1}}. \quad (27)$$

Finally, the free energy of the system is

$$F = -\frac{T}{N m_0} \log Z, \quad (28)$$

where we multiply by T/m_0 which is the effective temperature of metabasins.

We now suppose that a field h , conjugated to an observable O , is added to the Hamiltonian of the system which becomes $H' = H - hO$. One can show by a simple calculation that

$$\langle O \rangle = -\frac{dF}{dh} = -\sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} \frac{df_{\alpha_1}}{dh} = \langle \langle O_{\alpha_1} \rangle_1 \rangle_0, \quad (29)$$

where we defined $O_{\alpha_1} = -\frac{df_{\alpha_1}}{dh}$ the average of the observable O within the glassy state α_1 , $\langle \bullet \rangle_1$ the average over basins in a metabasin with weights w_{α_1} , $\langle \bullet \rangle_0$ the average over metabasins with weights w_{α_0} , and $\langle \bullet \rangle$ the total equilibrium average. The interpretation of Eq. (29) is straightforward: the total thermodynamic average of observable O in the Gibbs measure is obtained by first taking the average within each glassy basin, then taking the average over basins in a metabasin, and finally by taking the average over metabasins.

Taking another derivative, and defining as $\chi_{\alpha_1} = \frac{dO_{\alpha_1}}{dh} = -\frac{d^2 f_{\alpha_1}}{dh^2}$ the susceptibility inside state α_1 , we obtain

$$\begin{aligned} \chi &= \frac{d\langle O \rangle}{dh} = -\frac{d^2 F}{dh^2} = \sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} \frac{dO_{\alpha_1}}{dh} + \sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} \frac{dw_{\alpha_1|\alpha_0}}{dh} O_{\alpha_1} + \sum_{\alpha_0} \frac{dw_{\alpha_0}}{dh} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} O_{\alpha_1} \\ &= \langle \langle \chi_{\alpha_1} \rangle_1 \rangle_0 + \beta N m_1 \langle \langle O_{\alpha_1}^2 \rangle_1 - \langle O_{\alpha_1} \rangle_1^2 \rangle_0 + \beta N m_0 [\langle \langle O_{\alpha_1} \rangle_1^2 \rangle_0 - \langle \langle O_{\alpha_1} \rangle_1 \rangle_0^2] \\ &= \tilde{\chi}_2 + m_1 \tilde{\chi}_1 + m_0 \tilde{\chi}_0, \end{aligned} \quad (30)$$

where

$$\begin{aligned} \tilde{\chi}_2 &= \langle \langle \chi_{\alpha_1} \rangle_1 \rangle_0 = \sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} \frac{dO_{\alpha_1}}{dh}, \\ \tilde{\chi}_1 &= \beta N \langle \langle O_{\alpha_1}^2 \rangle_1 - \langle O_{\alpha_1} \rangle_1^2 \rangle_0 = \beta N \sum_{\alpha_0} w_{\alpha_0} \left[\sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} (O_{\alpha_1})^2 - \left(\sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} O_{\alpha_1} \right)^2 \right], \\ \tilde{\chi}_0 &= \beta N [\langle \langle O_{\alpha_1} \rangle_1^2 \rangle_0 - \langle \langle O_{\alpha_1} \rangle_1 \rangle_0^2] = \beta N \left[\sum_{\alpha_0} w_{\alpha_0} \left(\sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} O_{\alpha_1} \right)^2 - \left(\sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0} O_{\alpha_1} \right)^2 \right]. \end{aligned} \quad (31)$$

The interpretation of Eqs. (30) and (31) is also straightforward, and is illustrated in Fig. 1. The susceptibility $\tilde{\chi}_2$ is the average of the susceptibility of a given glass state χ_{α_1} over states: it represents the average susceptibility of basins. The term $\tilde{\chi}_1$ is given by the fluctuation of O_{α_1} from basin to basin inside a same metabasin (averaged over metabasins). Finally, the term $\tilde{\chi}_0$ is given by the fluctuation from metabasin to metabasin of the average of O within a metabasin, given by $\langle O_{\alpha_1} \rangle_1$. An equilibrium system is able to explore all the structure of basins and metabasins, therefore its susceptibility is given by the (properly weighted) sum of these three terms. Instead, a system that is completely stuck within a given glass basin will only receive contributions from the term $\tilde{\chi}_2$. A system that can explore one metabasin, but cannot escape from it, will have a susceptibility $\tilde{\chi}_2 + m_1 \tilde{\chi}_1$.

This construction is obviously generalized to k RSB. Recalling that $m_k = 1$ corresponds to the innermost basins, while levels $i < k$ corresponds to larger metabasins, we have that a system that can explore the state structure down to a level i has a susceptibility given by

$$\chi_i = \sum_{j=i}^k m_j \tilde{\chi}_j. \quad (32)$$

For $i = k$ we have the basin susceptibility, while for $i = 0$ we obtain the total susceptibility. Intermediate values of i correspond to partially confined systems.

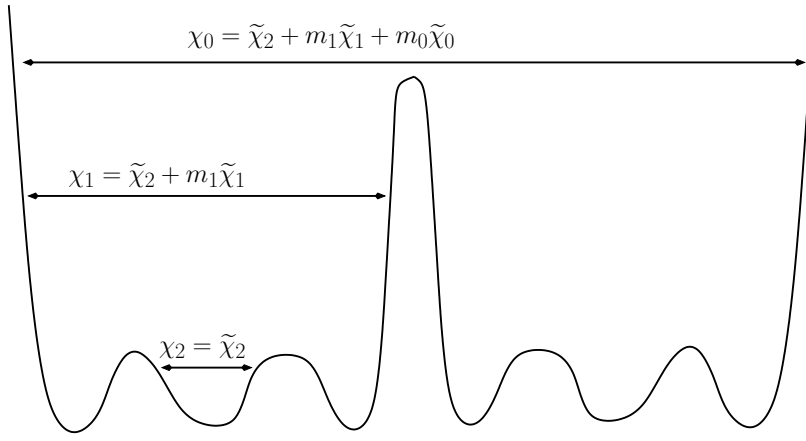


FIG. 1: An illustration of the susceptibilities associated to different levels of exploration of phase space in a 2RSB structure. A system confined in a single glass basin is characterized by the intra-state susceptibility $\chi_2 = \tilde{\chi}_2$. A system that can explore the first level of metabasins is characterized by $\chi_1 = \tilde{\chi}_2 + m_1 \tilde{\chi}_1$. Finally, a system that can explore the full equilibrium structure of all metabasins has the equilibrium susceptibility $\chi = \chi_0 = \tilde{\chi}_2 + m_1 \tilde{\chi}_1 + m_0 \tilde{\chi}_0$.

B. Computing the partial susceptibilities using the molecular liquid

We now discuss the connection with the molecular liquid computation of Sec. II. The molecular liquid provides a way to represent the partition function (27) [22, 36]. In a 2RSB ansatz, it is assumed that replicas arrange in groups of m_1 replicas, each group $B = 1 \cdots m_0/m_1$ being in the same state α_B . All replicas are assumed to be in the same metabasin, hence $\alpha_B \in \alpha_0$ for all B . Assuming that each replica is subject to a different field h_a , the partition function of the molecular liquid is

$$Z_{\text{ml}} = \sum_{\alpha_0} \prod_{B=1}^{m_0/m_1} \left(\sum_{\alpha_1 \in \alpha_0} e^{-\beta N \sum_{a \in B} f_{\alpha_1}(h_a)} \right). \quad (33)$$

and its free energy is

$$F_{\text{ml}} = -\frac{T}{N} \log Z_{\text{ml}}. \quad (34)$$

Note that here we do not divide by m_0 , which is natural because Z_{ml} is interpreted as the partition function of molecules at temperature T . In the limit $h_a \rightarrow 0$, we have

$$Z_{\text{ml}} = \sum_{\alpha_0} \prod_{B=1}^{m_0/m_1} \left(\sum_{\alpha_1 \in \alpha_0} e^{-\beta N m_1 f_{\alpha_1}} \right) = \sum_{\alpha_0} \left(\sum_{\alpha_1 \in \alpha_0} e^{-\beta N m_1 f_{\alpha_1}} \right)^{\frac{m_0}{m_1}}, \quad (35)$$

which coincides with Eq. (27).

A simple computation along the lines of the previous section allows one to compute the partial susceptibilities. We define

$$w_{\alpha_0} = \frac{1}{Z_{\text{ml}}} \prod_{B=1}^{m_0/m_1} \left(\sum_{\alpha_1 \in \alpha_0} e^{-\beta N \sum_{a \in B} f_{\alpha_1}(h_a)} \right), \quad (36)$$

$$w_{\alpha_1|\alpha_0}^B = \frac{e^{-\beta N \sum_{a \in B} f_{\alpha_1}(h_a)}}{\sum_{\alpha_1 \in \alpha_0} e^{-\beta N \sum_{a \in B} f_{\alpha_1}(h_a)}},$$

where w_{α_0} is the total weight for having all replicas in state α_0 , while $w_{\alpha_1|\alpha_0}^B$ is the weight for having the replicas of group B in state $\alpha_1 \in \alpha_0$. Taking a derivative of the free energy by h_a we find

$$-\frac{dF_{\text{ml}}}{dh_a} = \sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0}^{B(a)} O_{\alpha_1}(h_a), \quad (37)$$

where $B(a)$ represents the group which contains the replica a . We now take another derivative, and observe that $w_{\alpha_1|\alpha_0}^{B(a)}$ depends only on the fields h_b such that $b \in B(a)$, hence $\frac{dw_{\alpha_1|\alpha_0}^{B(a)}}{dh_b} \propto I_{ab}^{m_1}$. We find

$$-\frac{d^2 F_{\text{ml}}}{dh_a dh_b} = \delta_{ab} \sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0}^{B(a)} \chi_{\alpha_1}(h_a) + I_{ab}^{m_1} \sum_{\alpha_0} w_{\alpha_0} \sum_{\alpha_1 \in \alpha_0} \frac{dw_{\alpha_1|\alpha_0}^{B(a)}}{dh_b} O_{\alpha_1}(h_a) + \sum_{\alpha_0} \frac{dw_{\alpha_0}}{dh_b} \sum_{\alpha_1 \in \alpha_0} w_{\alpha_1|\alpha_0}^{B(a)} O_{\alpha_1}(h_a) . \quad (38)$$

Developing the derivatives and setting $h_a = 0$ it is easy to check that we obtain for the susceptibility matrix:

$$\chi_{ab} = - \left. \frac{d^2 F_{\text{ml}}}{dh_a dh_b} \right|_{h_a=0} = \tilde{\chi}_2 \delta_{ab} + \tilde{\chi}_1 I_{ab}^{m_1} + \tilde{\chi}_0 I_{ab}^{m_0} . \quad (39)$$

Recall that in the 2RSB case $m_2 = 1$ and $I_{ab}^{m_2} = \delta_{ab}$, the generalization to k RSB is straightforward:

$$\chi_{ab} = \sum_{i=0}^k \tilde{\chi}_i I_{ab}^{m_i} , \quad (40)$$

which shows that from the susceptibility matrix of the molecular liquid one can extract the partial susceptibilities $\tilde{\chi}_k$.

C. Shear modulus

In the case of the shear modulus, from Eq. (23) we deduce that

$$\begin{aligned} \beta \hat{\mu}_{ab} &= \sum_{i=0}^k \beta \tilde{\mu}_i I_{ab}^{m_i} , \\ \beta \tilde{\mu}_k &= \frac{1}{m \hat{\gamma}_k} , \\ \beta \tilde{\mu}_i &= -\frac{1}{m m_i} \left(\frac{1}{\hat{\gamma}_{i+1}} - \frac{1}{\hat{\gamma}_i} \right) , \quad i = 1, \dots, k-1 , \\ \beta \tilde{\mu}_0 &= -\frac{1}{m^2 \hat{\gamma}_1} . \end{aligned} \quad (41)$$

Note that $\tilde{\mu}_k$ is positive, as it corresponds to the intra-basin shear modulus, while all the other terms are *negative* (because $\hat{\gamma}_i$ is a monotonically decreasing function of increasing i [32]), which is correct because they represent the *softening* of the system due to the fact that it can explore more phase space.

From this result we can compute the total shear modulus $\hat{\mu}_i$ of a system that is able to explore the structure of metabasins down to level i . We place a hat on the shear modulus to remember that it has been scaled by $2/d$ as in Eq. (23). According to Eq. (32), we have for $i > 0$:

$$\beta \hat{\mu}_i = \sum_{j=i}^k m_j \beta \tilde{\mu}_j = \frac{1}{m \hat{\gamma}_k} + \sum_{j=i}^{k-1} \frac{1}{m} \left(\frac{1}{\hat{\gamma}_i} - \frac{1}{\hat{\gamma}_{i+1}} \right) = \frac{1}{m \hat{\gamma}_i} , \quad (42)$$

while, recalling that $m_0 = m$,

$$\beta \hat{\mu}_0 = \beta \hat{\mu}_1 - m_0 \frac{1}{m^2 \hat{\gamma}_1} = 0 , \quad (43)$$

which is correct because if the system can explore the whole phase space, then it is a liquid and has a zero shear modulus. Finally, note that in the fullRSB limit $k \rightarrow \infty$, $\hat{\mu}_i$ has a well defined limit, as it should be for physical quantities (while $\tilde{\mu}_i$ does not have a finite limit). The index i becomes a continuous index y [32] and we obtain

$$\beta \hat{\mu}(y) = \frac{1}{m \gamma(y)} . \quad (44)$$

IV. PREDICTIONS FOR PHYSICAL OBSERVABLES

Eqs. (42) and (44) are the main results of this paper, and we now derive their physical consequences, based on the phase diagram of hard spheres in $d \rightarrow \infty$ derived in [31, 32].

A. The dynamical transition

As shown in [31, 32], at the dynamical transition, where the glassy states first appear, the system is described by a 1RSB structure. Therefore, using [32, Eq.(113)], the shear modulus matrix has the following structure [6, 23]:

$$\beta \hat{\mu}_{ab} = \frac{1}{m \hat{\gamma}_1} \left(\delta_{ab} - \frac{1}{m} \right) = \frac{1}{\hat{\Delta}_1} \left(\delta_{ab} - \frac{1}{m} \right), \quad (45)$$

and the intra-state shear modulus is

$$\beta \hat{\mu}_{\text{EA}} \equiv \beta \hat{\mu}_1 = \frac{1}{\hat{\Delta}_1} \equiv \frac{1}{\hat{\Delta}_{\text{EA}}}. \quad (46)$$

We obtain therefore that the shear modulus is proportional to the inverse of the cage radius. This quantity jumps from $\hat{\Delta}_{\text{EA}} = \infty$ for $\hat{\varphi} < \hat{\varphi}_d$ in the liquid phase, to $\hat{\Delta}_{\text{EA}} \sim \hat{\Delta}_d - C(\hat{\varphi} - \hat{\varphi}_d)^{1/2}$ in the glass phase at $\hat{\varphi} > \hat{\varphi}_d$ [2]. Correspondingly, the shear modulus has a discontinuous jump at the dynamical transition, and behaves as

$$\beta \hat{\mu}_{\text{EA}}(\hat{\varphi}) \sim \beta \hat{\mu}_d + C'(\hat{\varphi} - \hat{\varphi}_d)^{1/2} \quad (47)$$

just above the glass transition. This result is consistent with the results of Mode-Coupling Theory [5] and previous computations using replicas [6, 24, 25]. The presence of a jump is consistent with the numerical results of [4] and the experimental results of [39], although the square root singularity cannot be easily observed numerically or experimentally due to the fact that the dynamical transition becomes a crossover in finite dimensions [3].

B. Scaling of the intra-state shear modulus around jamming

Around the jamming transition, the system is described by a fullRSB solution [32]. The intra-state shear modulus characterizes the behavior of a system which is completely confined in a glassy state. It is given, using [32, Eq.(113)], by

$$\beta \hat{\mu}_{\text{EA}} \equiv \beta \hat{\mu}_k = \frac{1}{m \hat{\gamma}_k} = \frac{1}{\hat{\Delta}_k} \equiv \frac{1}{\hat{\Delta}_{\text{EA}}}, \quad (48)$$

where $\hat{\Delta}_{\text{EA}}$ is the cage radius of the glass. Therefore, we obtain the prediction that the shear modulus is proportional to the inverse of the cage radius, and to temperature, as it should be for hard spheres where rigidity has an *entropic* origin [4]. It was shown in [32] that on approaching the jamming transition, $\hat{\Delta}_{\text{EA}} \sim p^{-\kappa}$, where p is the reduced pressure, whose inverse vanishes linearly with density on approaching jamming. We therefore predict that the shear modulus of the glass diverges on approaching the jamming transition of hard spheres as

$$\beta \hat{\mu}_{\text{EA}} \sim p^\kappa \sim |\varphi - \varphi_j|^{-\kappa}, \quad (49)$$

with the exponent $\kappa = 1.41575$ given in [32]. This result is also nicely consistent with the effective medium approach that has been developed in [16].

An extension of these results to soft harmonic spheres has been also discussed in [32]. In that case, when temperature goes to zero, one has $m = T/\tau$ with a finite τ , while $\hat{\gamma}_k$ remains finite. Therefore the shear modulus is finite, as it should be because in this case rigidity has a *mechanical* origin [4], and is given by

$$\hat{\mu}_{\text{EA}} = \frac{\tau}{\hat{\gamma}_k}. \quad (50)$$

Furthermore, according to the analysis of [32], on approaching jamming, $\tau \sim |\varphi - \varphi_j|$ vanishes linearly, and $\hat{\gamma}_k \sim \tau^{\kappa-1}$. We therefore obtain the prediction

$$\hat{\mu}_{\text{EA}} = \frac{\tau}{\hat{\gamma}_k} \sim \tau^{2-\kappa} \sim |\varphi - \varphi_j|^{2-\kappa}, \quad (51)$$

which is different from what has been argued in [15–17], where a scaling $\hat{\mu}_{\text{EA}} \sim |\varphi - \varphi_j|^{1/2}$ has been derived. Although the two predictions are quite close since $2 - \kappa = 0.58425$, they definitely differ, and the origin of this discrepancy remains to be clarified.

C. Exploring the metabasin: out of equilibrium dynamics

Another very interesting prediction of Eq. (44) is that if the system is allowed to explore a little bit the metabasin structure around a glass state, then the shear modulus changes dramatically. In fact, suppose that the system is able to explore the metabasins structure down to scale y . Then the effective shear modulus is given by Eq. (44) with some finite y . On approaching jamming, if y remains finite, then $\gamma(y)$ is also finite [32]. At the same time, $m \sim 1/p$ [32], and we conclude that the shear modulus scales with pressure as

$$\beta\hat{\mu}(y) = \frac{1}{m\gamma(y)} \sim p, \quad (52)$$

i.e. it scales with pressure with a different exponent than the intra-basin shear modulus. Since $\kappa > 1$, the metabasin shear modulus is much smaller than the intra-basin one: exploring a little bit the phase space makes the system much softer.

How can the system explore the metabasin structure? If the system is prepared at equilibrium in a glass state, then the barriers that need to be crossed to change state within a metabasin diverge with d as d^α with some exponent $\alpha < 1$, making the exploration of phase space impossible. This is also the case if the glass is prepared through a slow annealing: in this case at the end of the annealing the system is stuck into a glass and cannot escape from it. In that case the relevant quantity is $\hat{\mu}_{\text{EA}}$ discussed above. However, if the system is prepared by a fast quench from the liquid into the glass phase at time 0, and its evolution is recorded as a function of the waiting time t_w after the quench, then it can explore a bit the metabasin structure before getting stuck into a glass [40]. Suppose that we let the system age after the quench for a time t_w , and at time t_w we add a small strain γ to measure the shear modulus, $\mu(t, t_w) = \sigma(t, t_w)/\gamma$, where $\sigma(t, t_w)$ is the stress at time t . The evolution of $\mu(t, t_w)$ is illustrated in Fig. 2. We expect that at short $t - t_w$, $\mu(t, t_w)$ reaches a plateau at $\mu(t, t_w) \sim \hat{\mu}_{\text{EA}} \sim p^\kappa$. At larger times $t \sim \tau_{\text{mb}}(t_w)$, the system can explore neighboring glass basins [40], and $\mu(t, t_w)$ should drop to a second plateau corresponding to $\hat{\mu}(y)$ for some finite y , hence $\mu(t, t_w) \sim \hat{\mu}(y) \sim p$ at longer times. The scaling $\mu \sim p$ is captured by the 1RSB solution [24, 25]. Note that at *much* longer times $t \sim \tau_\alpha(t_w)$, $\mu(t, t_w)$ will eventually drop to zero. The two time scales $\tau_{\text{mb}}(t_w)$ and $\tau_\alpha(t_w)$ certainly grow with t_w , but their scaling is still unclear. It is reasonable to expect that $\tau_{\text{mb}}(t_w)$, that is the time needed to cross barriers between basins inside a same metabasin, will grow as a power-law of t_w [40]. The time scale $\tau_\alpha(t_w)$ is associated to crossing the largest barriers, those separating the largest metabasins; its scaling with t_w is not clear and it might be much faster above some critical pressure [41].

A numerical study of aging close to jamming has been performed in [25], and the results are consistent with these predictions. However, a more accurate numerical study should be performed to make a precise comparison with the theory. Note that a scaling of the shear modulus $\mu \sim p$ has been reported in a previous experiment [14].

D. Reparametrization invariance

A more stringent test of the theory can be performed by looking at the so-called *reparametrization invariant* regime of the out-of-equilibrium dynamics after a quench. Suppose that we perform the aging experiment described above, and starting from a time t_w after the quench, we measure both the mean square displacement $\Delta(t, t_w) = N^{-1} \sum_i \langle [x_i(t) - x_i(t_w)]^2 \rangle$ and the shear modulus $\mu(t, t_w)$. After a short transient, both quantities reach their asymptotic values inside a glass basin, hence $\Delta(t, t_w) \sim \hat{\Delta}_{\text{EA}}$ and $\mu(t, t_w) \sim \hat{\mu}_{\text{EA}}$. For large t_w , and at larger times $t \sim \tau_{\text{mb}}(t_w)$, the dynamics enter in a *reparametrization invariant* regime [40]. In this regime, larger and larger groups of states are explored *in a restricted equilibrium*. Hence, $\Delta(t, t_w) \sim \Delta(y)$ and $\mu(t, t_w) \sim \hat{\mu}(y)$ with the same value of y that is dynamically selected. One can then eliminate time t parametrically from the dynamical data to obtain a curve $\hat{\mu}(\Delta, t_w)$. The same can be done in the replica result by eliminating y parametrically to obtain a curve $\hat{\mu}(\Delta)$. Based on general results obtained in the context of spin glasses [40], one expects that

$$\lim_{t_w \rightarrow \infty} \hat{\mu}(\Delta, t_w) = \hat{\mu}(\Delta), \quad (53)$$

provided in the replica calculation the parameter m is selected to be on the *threshold line* [32, 40] corresponding to the pressure at which the dynamics is investigated.

The replica prediction is that

$$\frac{\beta\hat{\mu}(\Delta)}{p} \propto \beta m \hat{\mu}(\Delta) = \frac{1}{\gamma(\Delta)}, \quad (54)$$

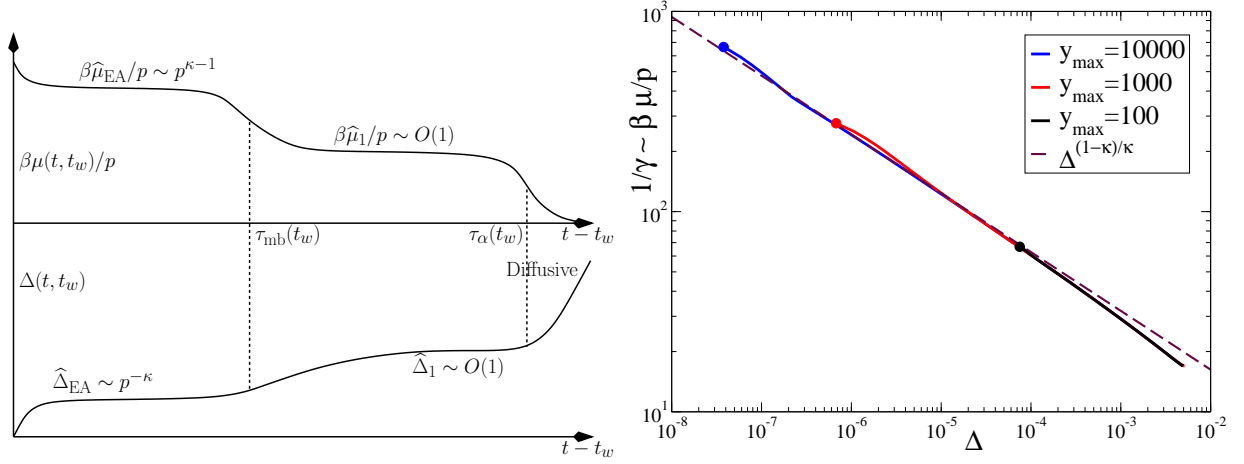


FIG. 2: (Left) Schematic evolution of the shear modulus $\mu(t, t_w)$ and the mean square displacement $\Delta(t, t_w)$, for a large time t_w after a quench, as a function of $t - t_w$. (Right) The function $\frac{\beta\hat{\mu}(\Delta)}{p} \sim 1/\gamma(\Delta)$ that characterizes the reparametrization invariant regime, obtained from the numerical solution of the fullRSB equations [32]. The dots mark the intra-state point $(\hat{\Delta}_{EA}, \beta\hat{\mu}_{EA}/p)$. The three curves correspond to different cutoffs $y_{\max} \propto p$. The slight bending of the curves around the dots is an artifact of the numerical computation [32].

and because $\Delta(y) \sim y^{-\kappa}$ and $\gamma(y) \sim y^{-\kappa+1}$ for $y \rightarrow \infty$, we have that for $\Delta \rightarrow 0$, $\frac{\beta\hat{\mu}(\Delta)}{p} \sim 1/\gamma(\Delta) \sim \Delta^{(1-\kappa)/\kappa}$. In other words, in the jamming limit $p \rightarrow \infty$, $\beta\hat{\mu}(\Delta)$ is proportional to reduced pressure, in such a way that $\frac{\beta\hat{\mu}(\Delta)}{p}$ tends to a master function. At finite pressure, this master function is defined in an interval $\Delta \in [\hat{\Delta}_{EA}, \hat{\Delta}_1]$. For large pressures, $\hat{\Delta}_{EA} \sim p^{-\kappa}$ goes to zero, while $\hat{\Delta}_1$ stays finite. Correspondingly the shorter time plateau of the shear modulus diverges faster than p , leading to the divergent behavior of the master function, $\frac{\beta\hat{\mu}(\Delta)}{p} \sim \Delta^{(1-\kappa)/\kappa}$. An illustrative example, obtained from the numerical data of [32] for $\gamma(y)$ and $\Delta(y)$, is given in Fig. 2.

V. CONCLUSIONS

By means of the exact solution of amorphous infinite-dimensional hard spheres [30–32], we are able to compute the shear modulus in the whole phase diagram. We found that in $d \rightarrow \infty$ the intra-state shear modulus is simply given by Eq. (48), $\hat{\mu}_{EA} = T/\hat{\Delta}_{EA}$ and is equal to temperature divided by the cage radius (Debye-Waller factor) of the glass. This formula predicts that, at the dynamical transition, $\hat{\mu}_{EA}$ jumps from zero to a finite value, followed by a square-root singularity, according to Eq. (47). Moreover, it predicts that around the jamming transition $\hat{\mu}_{EA}$ has critical scalings, described in Sec. IV B, with critical exponents that are predicted analytically [32]. These results provide a comprehensive picture of the rheology of complex amorphous fluids [4] and agree with previous analytical results obtained using MCT [5, 7], replicas [6, 24] and effective medium [16, 17] approaches. We are able to unify these different approaches and put them on a firm theoretical basis, thanks to the fact that the method is exact for $d \rightarrow \infty$.

We also analyzed the behavior of the inter-state shear moduli, that characterize the behavior of the system in situations where it is not confined in a single glass basin, but can also explore neighboring states within larger metabasins. This can happen for example during the out-of-equilibrium dynamics after a sudden deep quench. An interesting result is that the inter-state shear modulus has a different scaling with pressure on approaching jamming, $\beta\hat{\mu}(y) \sim p \ll p^\kappa \sim \beta\hat{\mu}_{EA}$. This means that if the system is able to explore a little bit of phase space beyond a single glass basin, its rigidity is decreased dramatically. This effect, which is a new prediction, could be detected in numerical simulations and experiments [25]. We have also discussed the possibility of constructing reparametrization-invariant parametric plots of different observables [40], a procedure that should allow one to probe the fullRSB structure of the states close to jamming. Finally, let us recall that the notions of basins and metabasins were proposed within the energy landscape picture of structural glasses [42], which naturally implies a hierarchy of rigidities [6].

There are several points that should be discussed further. First of all, one could extend this approach to finite dimensional systems [2, 6, 22]. In that case the method is of course approximate, but the qualitative picture (including the scaling properties) is unchanged and the method provides good quantitative estimates of physical observables,

the equation of state of the glass [2, 22] and the different transition densities or temperatures. This will be useful to perform more direct comparisons between the theory and numerical simulations [4] or experiments [14, 39]. Most importantly, the discrepancy between the present approach and an effective medium computation [15–17] in the case of harmonic soft spheres should be resolved. Of course, most of the conclusions of Ref. [32] about the fullRSB solution (e.g. how it is affected by critical fluctuations in finite dimensions) also apply to the present work.

Acknowledgments

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Appendix A: Fluctuation formula for the shear modulus

1. Fluctuation formula

In this section we provide an alternative derivation of Eq. (15) based on the fluctuation formula for the shear modulus matrix that has been derived in [6] and reads

$$N\mu_{ab} = \sum_{i<j} \langle \mu_{ij}^a \rangle \delta_{ab} - \beta \left(\sum_{i<j, k<l} \langle \sigma_{ij}^a \sigma_{kl}^b \rangle - \langle \sigma_{ij}^a \rangle \langle \sigma_{kl}^b \rangle \right), \quad (\text{A1})$$

where indexes $i, j, k, l = 1, \dots, N$ run on the molecules of the system, the averages are on the Boltzmann distribution of the molecular liquid and

$$\begin{aligned} \mu_{ij}^a &= \mu^a(x_{ai} - x_{aj}) = \frac{\partial^2}{\partial \gamma_a^2} v(|S(\gamma_a)(x_{ai} - x_{aj})|) \Big|_{\gamma_a=0}, \\ \sigma_{ij}^a &= \sigma^a(x_{ai} - x_{aj}) = \frac{\partial}{\partial \gamma_a} v(|S(\gamma_a)(x_{ai} - x_{aj})|) \Big|_{\gamma_a=0}. \end{aligned} \quad (\text{A2})$$

This formula can be derived by considering the molecular liquid in the canonical ensemble, without introducing the density field $\rho(\vec{x})$, and taking the second derivative with respect to shear.

We now introduce a molecular version of the usual n -point density functions [43], which are defined as

$$\rho^{(n)}(\vec{x}_1 \cdots \vec{x}_n) = \sum_{i_1 \neq i_2 \neq \cdots \neq i_n} \langle \delta(\vec{x}_{i_1} - \vec{x}_1) \cdots \delta(\vec{x}_{i_n} - \vec{x}_n) \rangle, \quad (\text{A3})$$

and give the probability of finding n molecules in positions $\vec{x}_1 \cdots \vec{x}_n$. In terms of these objects, and introducing functions $\mu^a(\vec{x}, \vec{y}) = \mu^a(x_a - y_a)$ and $\sigma^a(\vec{x}, \vec{y}) = \sigma^a(x_a - y_a)$, we have, as in standard liquid theory [43]:

$$\begin{aligned} \sum_{i<j} \langle \mu_{ij}^a \rangle &= \frac{1}{2} \int d\vec{x} d\vec{y} \rho^{(2)}(\vec{x}, \vec{y}) \mu^a(\vec{x}, \vec{y}), \\ \sum_{i<j} \langle \sigma_{ij}^a \rangle &= \frac{1}{2} \int d\vec{x} d\vec{y} \rho^{(2)}(\vec{x}, \vec{y}) \sigma^a(\vec{x}, \vec{y}), \\ \sum_{i<j, k<l} \langle \sigma_{ij}^a \sigma_{kl}^b \rangle &= \frac{1}{2} \int d\vec{x} d\vec{y} \rho^{(2)}(\vec{x}, \vec{y}) \sigma^a(\vec{x}, \vec{y}) \sigma^b(\vec{x}, \vec{y}) \\ &\quad + \int d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 \rho^{(3)}(\vec{x}_1, \vec{x}_2, \vec{x}_3) \sigma^a(\vec{x}_1, \vec{x}_2) \sigma^b(\vec{x}_1, \vec{x}_3) \\ &\quad + \frac{1}{4} \int d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 d\vec{x}_4 \rho^{(4)}(\vec{x}_1, \vec{x}_2, \vec{x}_3, \vec{x}_4) \sigma^a(\vec{x}_1, \vec{x}_2) \sigma^b(\vec{x}_3, \vec{x}_4). \end{aligned} \quad (\text{A4})$$

We now make use of the fact that, according to the analysis of [38, 44] in the limit $d \rightarrow \infty$, many-body correlations factor in products of two body correlations, and moreover the two-body correlation is given by its first virial contribution. Equivalently one can say that all n -point functions are given by their lowest order virial contribution, which is [45]:

$$\rho^{(n)}(\bar{x}_1 \cdots \bar{x}_n) = \prod_{i=1}^n \rho(\bar{x}_i) \prod_{i < j}^{1,n} e^{-\beta v(\bar{x}_i, \bar{x}_j)} , \quad (\text{A5})$$

where

$$e^{-\beta v(\bar{x}, \bar{y})} = \prod_{a=1}^m e^{-\beta v(x_a - y_a)} \quad (\text{A6})$$

is the replicated interaction potential.

Using this, we get

$$\begin{aligned} N\mu_{ab} = & \frac{1}{2} \int d\bar{x} d\bar{y} \rho(\bar{x}) \rho(\bar{y}) e^{-\beta v(\bar{x}, \bar{y})} [\mu^a(\bar{x}, \bar{y}) \delta_{ab} - \beta \sigma^a(\bar{x}, \bar{y}) \sigma^b(\bar{x}, \bar{y})] \\ & - \beta \int d\bar{x}_1 d\bar{x}_2 d\bar{x}_3 \rho(\bar{x}_1) \rho(\bar{x}_2) \rho(\bar{x}_3) e^{-\beta v(\bar{x}_1, \bar{x}_2)} e^{-\beta v(\bar{x}_2, \bar{x}_3)} e^{-\beta v(\bar{x}_3, \bar{x}_1)} \sigma^a(\bar{x}_1, \bar{x}_2) \sigma^b(\bar{x}_1, \bar{x}_3) \\ & - \frac{\beta}{4} \int d\bar{x}_1 d\bar{x}_2 d\bar{x}_3 d\bar{x}_4 \prod_{i=1}^4 \rho(\bar{x}_i) \left[\prod_{i < j}^{1,4} e^{-\beta v(\bar{x}_i, \bar{x}_j)} - e^{-\beta v(\bar{x}_1, \bar{x}_2)} e^{-\beta v(\bar{x}_3, \bar{x}_4)} \right] \sigma^a(\bar{x}_1, \bar{x}_2) \sigma^b(\bar{x}_3, \bar{x}_4) \end{aligned} \quad (\text{A7})$$

It is easy to show that the last two lines of the previous equation vanish in $d \rightarrow \infty$. Consider for example the three-body term. The integral is dominated by configurations where $\bar{x}_1 - \bar{x}_2 \sim D$ is orthogonal to $\bar{x}_1 - \bar{x}_3 \sim D$, so that \bar{x}_1 and \bar{x}_3 are far away and $e^{-\beta v(\bar{x}_3, \bar{x}_1)} \sim 1$ and can be neglected. The remaining integral can be evaluated through a saddle point and at leading order it is equal to the square of the average of σ^a , which vanishes in an isotropic liquid. Similarly, the last line is dominated by configurations where e.g. 1 and 3 overlap, 1 and 2 (and 3 and 4) are at distance $\sim D$, and 2 and 4 are far away. Again at this leading order one obtains the square of the average of σ^a , which vanishes. This analysis is consistent with the general principle that all contributions to thermodynamic averages coming from n -body correlation for $n > 2$ vanish in high dimensions [44]. Since the only two body contribution in the second and third line of Eq. (A7) is the average of σ^a which is zero, these contributions must vanish.

We obtain

$$\mu_{ab} = \frac{1}{2N} \int d\bar{x} d\bar{y} \rho(\bar{x}) \rho(\bar{y}) e^{-\beta v(\bar{x}, \bar{y})} [\mu^a(\bar{x}, \bar{y}) \delta_{ab} - \beta \sigma^a(\bar{x}, \bar{y}) \sigma^b(\bar{x}, \bar{y})] , \quad (\text{A8})$$

and inserting the explicit expressions of μ^a and σ^a it is easy to check that this expression becomes

$$\beta \mu_{ab} = -\frac{1}{2N} \int d\bar{x} d\bar{y} \rho(\bar{x}) \rho(\bar{y}) (x_{a2} - y_{a2})(x_{b2} - y_{b2}) \frac{\partial^2 f}{\partial x_{a1} \partial x_{b1}}(\bar{x} - \bar{y}) , \quad (\text{A9})$$

where f is the usual replicated Mayer function in absence of strain [30], corresponding to Eq. (4) for $\gamma_a = 0$. We now take into account translational invariance following the discussion of [30]. We introduce coordinates $u_a = x_a - X$ with $X = m^{-1} \sum_a x_a$, and we use that $\rho(\bar{x})$ does not depend on X , to obtain, following the notations of [30]:

$$\beta \mu_{ab} = -\frac{1}{2\rho} \int dX \mathcal{D}\bar{u} \mathcal{D}\bar{v} \rho(\bar{u}) \rho(\bar{v}) (X_2 + u_{a2} - v_{a2})(X_2 + u_{b2} - v_{b2}) \frac{\partial^2 f}{\partial u_{a1} \partial u_{b1}}(X + \bar{u} - \bar{v}) . \quad (\text{A10})$$

2. Simplifications for $d \rightarrow \infty$

We now make use of the results of [30, Sec. 5], that show that the integral in Eq. (A10) is dominated by the region where $u_a \sim v_a \sim d^{-1/2}$, while X is decomposed in a $(d - m)$ -component vector X_\perp , orthogonal to the plane defined by $\bar{u} - \bar{v}$, that is of order D , and a m -component vector $X_\parallel \sim d^{-1/2}$. This structure allows us to perform a series of crucial simplifications of Eq. (A10). It is clear, in fact, that with probability going to 1 for $d \rightarrow \infty$ with respect to the random choice of \bar{u}, \bar{v} according to the probability density $\rho(\bar{u})\rho(\bar{v})$, the direction $\mu = 2$ is orthogonal to all the vectors u_a and v_a , and therefore we can neglect the terms u_{a2} and v_{a2} in Eq. (A10). This is further supported

by the fact that the vectors u_a and v_a are small in the limit $d \rightarrow \infty$ while $X = X_\perp + X_\parallel$ remains of order 1 in most directions. We therefore obtain

$$\beta\mu_{ab} = -\frac{1}{2\rho} \int \mathcal{D}\bar{u}\mathcal{D}\bar{v}\rho(\bar{u})\rho(\bar{v}) \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \int dX (X_2)^2 f(X + \bar{u} - \bar{v}) \quad (\text{A11})$$

We now observe that direction $\mu = 2$ is equivalent to any other direction $\mu > 1$, because the strain has been eliminated and we are now considering an isotropic system. Direction $\mu = 1$ is still special due to the presence of the derivative, but we can consider this as a $1/d$ correction, therefore we can write

$$\beta\mu_{ab} = -\frac{1}{2\rho} \int \mathcal{D}\bar{u}\mathcal{D}\bar{v}\rho(\bar{u})\rho(\bar{v}) \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \frac{1}{d} \int dX X^2 f(X + \bar{u} - \bar{v}) , \quad (\text{A12})$$

and, recalling once again that $X = X_\perp + X_\parallel$ with $X_\perp \sim D$ and $X_\parallel \sim d^{-1/2}$, we have at leading order

$$\beta\mu_{ab} = -\frac{1}{2\rho} \int \mathcal{D}\bar{u}\mathcal{D}\bar{v}\rho(\bar{u})\rho(\bar{v}) \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \frac{1}{d} \int dX X_\perp^2 f(X + \bar{u} - \bar{v}) , \quad (\text{A13})$$

Now we specialize to the case of hard spheres, and following exactly the same steps of [30, Sec. 5, Eqs.(31)-(33)], we obtain

$$\int dX X_\perp^2 f(X + \bar{u}) = -V_d D^d \frac{\int d^m X_\parallel \Theta_{d-m+2}(D^2 - \min_a |X_\parallel + u_a|^2)}{\int d^m X_\parallel \Theta_{d-m}(D^2 - |X_\parallel|^2)} . \quad (\text{A14})$$

Next, following the steps of [30, Sec. 5.2], and introducing x_a by $u_a = x_a D / \sqrt{d}$, we obtain

$$\int dX X_\perp^2 f(X + \bar{u}) = -V_d D^{d+2} \frac{\int d^m \epsilon e^{-\frac{1}{2} \min_a |\epsilon + x_a|^2}}{\int d^m \epsilon e^{-\frac{1}{2} |\epsilon|^2}} = -V_d D^{d+2} \mathcal{F}(\bar{x}) = -V_d D^{d+2} \mathcal{F}\left(\frac{\sqrt{d}}{D} \bar{u}\right) , \quad (\text{A15})$$

and

$$\beta\mu_{ab} = \frac{V_d D^{d+2}}{2\rho d} \int \mathcal{D}\bar{u}\mathcal{D}\bar{v}\rho(\bar{u})\rho(\bar{v}) \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}\left(\frac{\sqrt{d}}{D} (\bar{u} - \bar{v})\right) . \quad (\text{A16})$$

3. Saddle point evaluation

It has been shown in [30] that for $d \rightarrow \infty$, integrals such as (A16) are dominated by a saddle point on \bar{u} and \bar{v} , due to the fact that $\rho(\bar{u})$ is exponential in d . Because the function \mathcal{F} is not exponential in d , it does not contribute to the saddle point. Because $\int \mathcal{D}\bar{u}\rho(\bar{u}) = \rho$, we obtain, recalling that $\rho V_d D^d = 2^d \varphi = d\hat{\varphi}$ where φ is the packing fraction and $\hat{\varphi}$ a scaled packing fraction,

$$\beta\mu_{ab} = \frac{\rho V_d D^{d+2}}{2d} \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}\left(\frac{\sqrt{d}}{D} (\bar{u}^{\text{sp}} - \bar{v}^{\text{sp}})\right) = \frac{\hat{\varphi} D^2}{2} \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}\left(\frac{\sqrt{d}}{D} (\bar{u}^{\text{sp}} - \bar{v}^{\text{sp}})\right) . \quad (\text{A17})$$

The function \mathcal{F} is rotationally invariant, hence it depends only on $(u_a - v_a) \cdot (u_b - v_b)$. We can choose any values of \bar{u}^{sp} and \bar{v}^{sp} , provided they respect the saddle point equations, which state [30] that $u_a \cdot u_b = q_{ab}$, $v_a \cdot v_b = p_{ab}$, and $u_a \cdot v_b = 0$, hence $(u_a - v_a) \cdot (u_b - v_b) = q_{ab} + p_{ab}$. We have that $\hat{q} = \hat{p}$, however when we take the derivative with respect to u_a we should only derive \hat{q} and not \hat{p} . We can simplify this by writing

$$\beta\mu_{ab} = \frac{\hat{\varphi} D^2}{2} \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}\left(\frac{d}{D^2} (\hat{q}_{ab} + \hat{p}_{ab})\right) \Big|_{\hat{p}=\hat{q}} = \frac{\hat{\varphi} D^2}{4} \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}\left(2\frac{d}{D^2} \hat{q}_{ab}\right) . \quad (\text{A18})$$

Also, following [31, 32] we can introduce the matrix

$$\Delta_{ab} = \frac{d}{D^2} (u_a - u_b)^2 = \frac{d}{D^2} (q_{aa} + q_{bb} - 2q_{ab}) , \quad (\text{A19})$$

and we have, following the definitions of [32], that

$$\beta\mu_{ab} = \frac{\hat{\varphi}D^2}{4} \frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}(\hat{\Delta}) , \quad (\text{A20})$$

with $\mathcal{F}(\hat{\Delta})$ given in [32]. We have then

$$\frac{\partial}{\partial u_{a1}} \mathcal{F}(\hat{\Delta}) = \frac{d}{D^2} \sum_{c(\neq a)} 2(u_{a1} - u_{c1}) \frac{\partial \mathcal{F}}{\partial \Delta_{ac}} , \quad (\text{A21})$$

and

$$\frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}(\hat{\Delta}) = \frac{d}{D^2} \times \begin{cases} 2 \sum_{c(\neq a)} \frac{\partial \mathcal{F}}{\partial \Delta_{ac}} + \sum_{c(\neq a), d(\neq a)} \frac{\partial^2 \mathcal{F}}{\partial \Delta_{ac} \partial \Delta_{ad}} 4 \frac{d}{D^2} (u_{a1} - u_{c1})(u_{a1} - u_{d1}) & \text{for } a = b \\ -2 \frac{\partial \mathcal{F}}{\partial \Delta_{ab}} + \sum_{c(\neq a), d(\neq b)} \frac{\partial^2 \mathcal{F}}{\partial \Delta_{ac} \partial \Delta_{bd}} 4 \frac{d}{D^2} (u_{a1} - u_{c1})(u_{b1} - u_{d1}) & \text{for } a \neq b \end{cases} \quad (\text{A22})$$

In each line of the previous equation, the second term is a factor $1/d$ smaller than the first, because it contains terms like $\frac{d}{D^2} u_{a1}^2 = \frac{d}{D^2} q_{aa}/d \propto \Delta/d$, hence it can be neglected. We obtain

$$\frac{\partial^2}{\partial u_{a1}\partial u_{b1}} \mathcal{F}(\hat{\Delta}) = \frac{2d}{D^2} \left[\delta_{ab} \sum_{c(\neq a)} \frac{\partial \mathcal{F}}{\partial \Delta_{ac}} - (1 - \delta_{ab}) \frac{\partial \mathcal{F}}{\partial \Delta_{ab}} \right] , \quad (\text{A23})$$

and using this we obtain our final result

$$\beta\mu_{ab} = \frac{d}{2} \hat{\varphi} \left[\delta_{ab} \sum_{c(\neq a)} \frac{\partial \mathcal{F}}{\partial \Delta_{ac}} - (1 - \delta_{ab}) \frac{\partial \mathcal{F}}{\partial \Delta_{ab}} \right] , \quad (\text{A24})$$

which coincides with Eq. (15).

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